More Accurate Modeling of Heat Transfer in Internal Combustion Engines (ACE145)

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DOE Vehicle Technologies Office Annual Merit Review
2 June 2020

This research was conducted as part of the Partnership to Advance Combustion Engines (PACE) sponsored by the U.S. Department of Energy (DOE) Vehicle Technologies Office (VTO). A special thanks to DOE VTO program managers Mike Weismiller and Gurpreet Singh.

Overview

Timeline

- **PACE started FY2019 Q3**
- **Proposed as 5-yr project under DOE lab call (~25% complete)**
  - Focus and objectives of tasks will be adjusted
- **Overall PACE work plan discussed in ACE 138**

FY2019	FY2020		FY2021	FY2022	FY2023

Budget

PI	Task	FY2019	FY2020
Edwards, ORNL	B.02.01 Cold-start simulation efforts	$200k*	$350k*
Wissink, ORNL	B.01.01 Neutronic engine	$1009k**	$100k
Pickett, SNL	D.01.04, D.01.05 HT-focused spray experiments	$380k*	$380k*

* Efforts under these tasks are split across multiple presentations

** One-time funding for hardware purchase

Barriers

- **U.S. DRIVE Advanced Combustion and Emission Control Roadmap**
  - Understand and improve dilute combustion strategies during cold start and cold operation to reduce emissions.
  - Understanding and robust modeling tools for rapidly screening proposed designs based on sound metrics are lacking.
- **PACE Major Outcome 8**
  - Deeper understanding of cold-start physics and chemistry in combustion system, hot-end exhaust, and aftertreatment to achieve faster, numerically aided design and calibration.

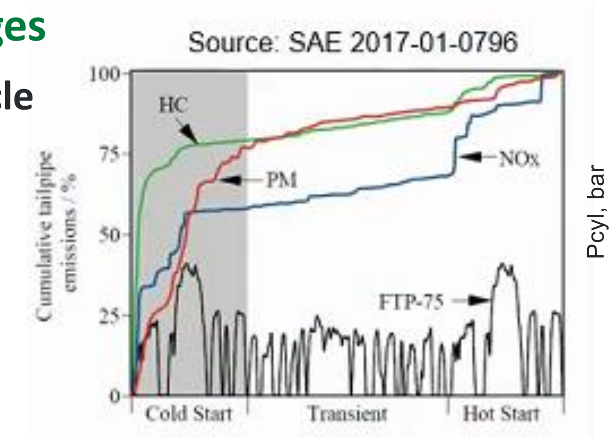
Partners

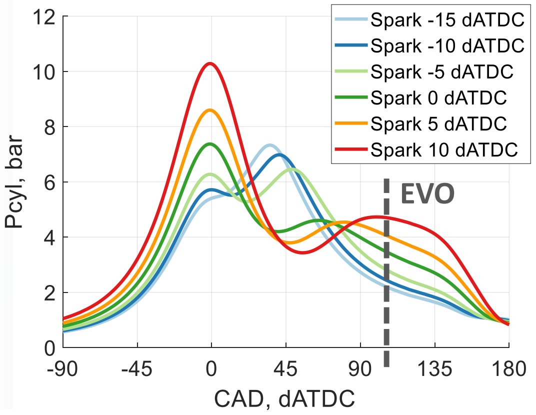
- **PACE is a DOE-funded consortium of 6 National Labs working toward common objectives (ACE 138)**
  - Goals and work plan developed with input from stakeholders including DOE, ACEC Tech Team, commercial CFD vendors, et al.
- **Specific partners on the work shown here…**
  - Edwards: LLNL, ANL, LANL, SNL, Convergent Science, GM
  - Wissink: SwRI, ORNL Spallation Neutron Source and Neutron Sciences Directorate
  - Pickett: ORNL, ECN Spray G (20+ partners), SNL modeling
  - Additional details on later slides…

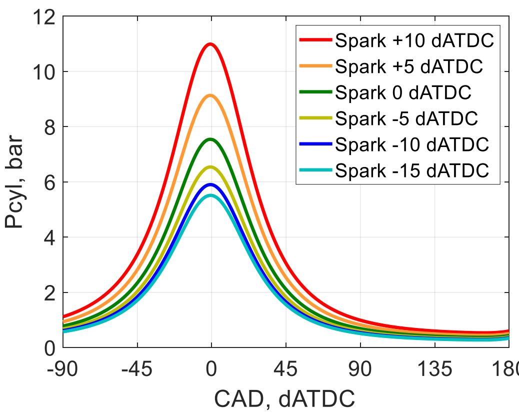
Relevance

Cold-start presents numerous challenges

- **Majority of emissions over FTP drive cycle produced during catalyst warm-up**
- **Catalyst heating strategies often involve late heat release for hotter exhaust**
- **Conventional modeling approaches struggle to accurately capture behavior**

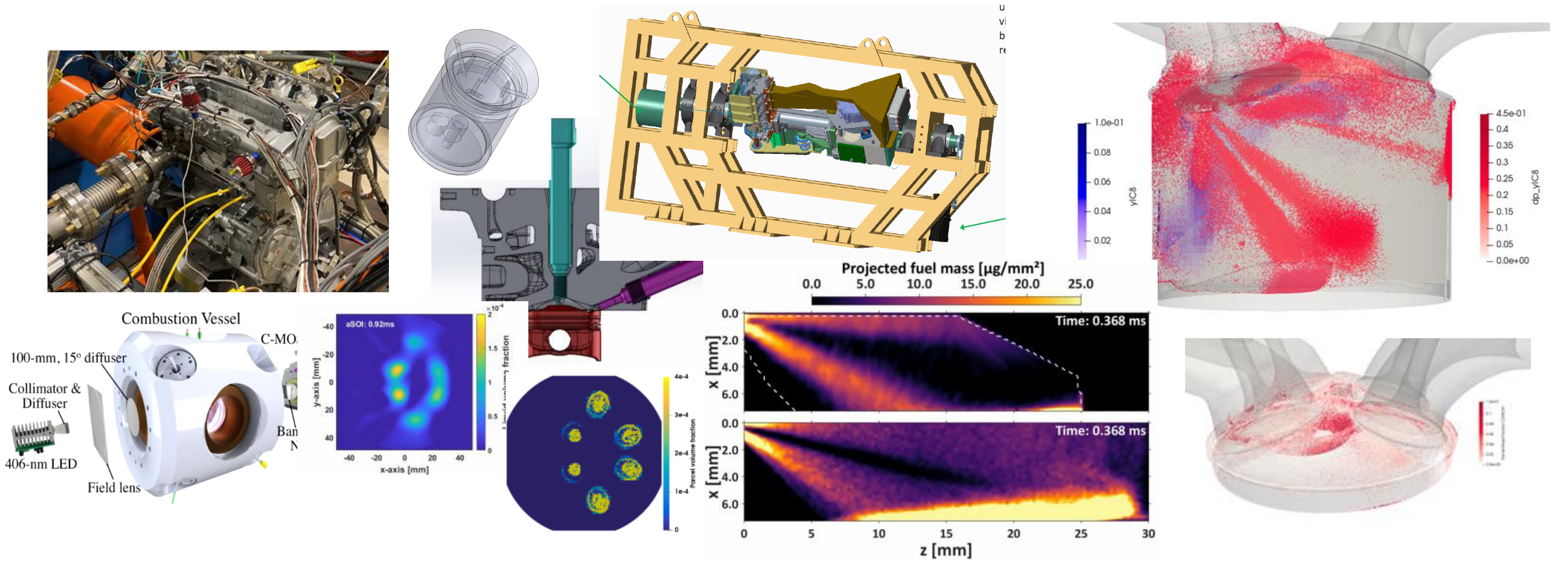






PACE using a multi-faceted approach

- **Builds on recent studies**
  - GM, UWisc, MIT, et al.
- **Fundamental experiments to develop understanding and validation data**
- **Development of improved sub-models**
- **Integration to highly-detailed CFD models**

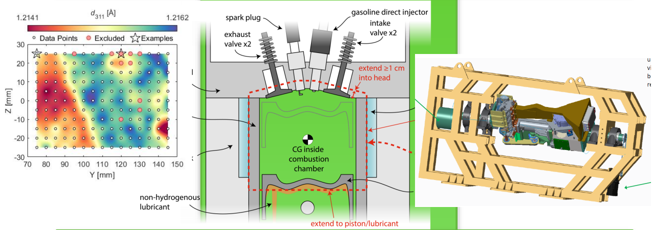


<u>PACE Major Outcome 8:</u> Deeper understanding of cold-start physics & chemistry to achieve faster, numerically-aided design & calibration

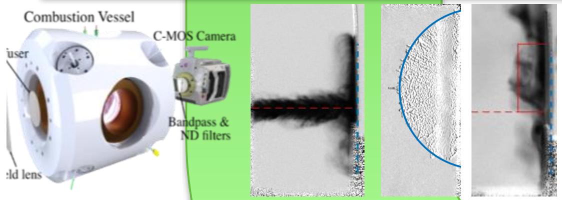
Overall Approach

Experimental Efforts

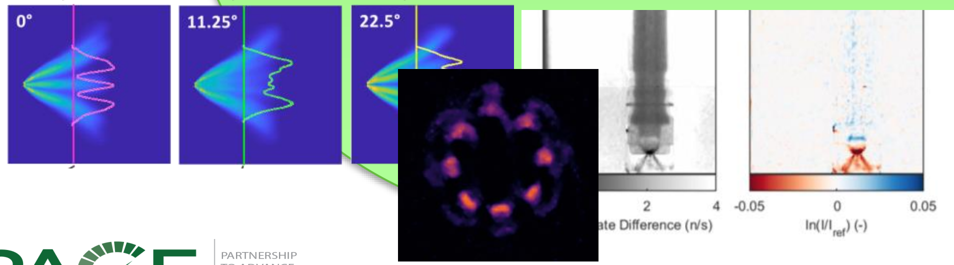
Neutron diffraction for *in situ* measurements in an operating engine
B.01.01 (PI: Wissink, ORNL)



Spray-wall impingement with film formation and soot quantification
D.01.05 (PI: Pickett, SNL)
D.01.04 (PI: Manin, SNL)



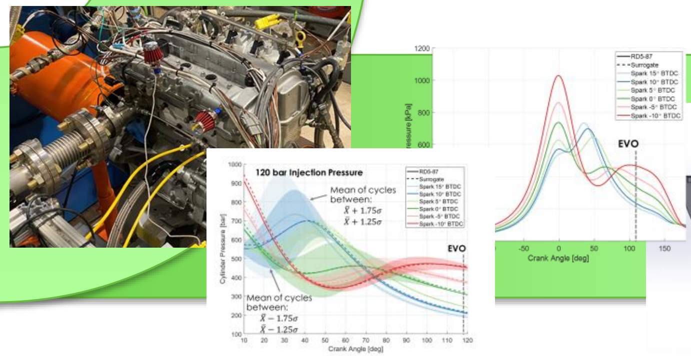
Spray imaging (ACE 143, Powell & ACE 144, Pickett)



Submodel Development

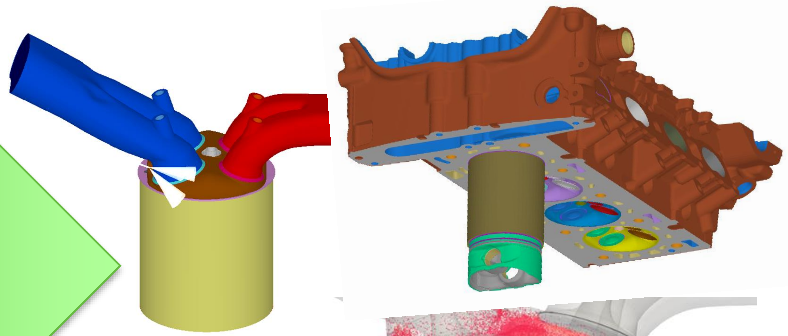
Kinetics and flame speed tables (ACE 139, Wagnon)
Conjugate heat transfer (CHT)
Injector settings
Corrected Distortion spray model (ACE 144, Pickett)
Spray models (ACE 143, Powell; FT 069 Splitter)
Wall and film models (ACE 144, Pickett)
Ignition models (ACE 142, Scarcelli)
Soot models and mechanisms (ACE 144, Pickett)
Flow solvers (ACE 146, Ameen)
Faster solvers (ACE 140, Whitesides)
etc.

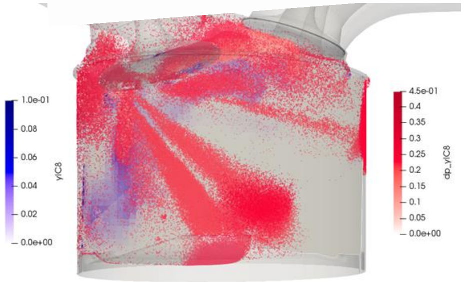
Cold-start engine experiments (ACE 149, Curran)

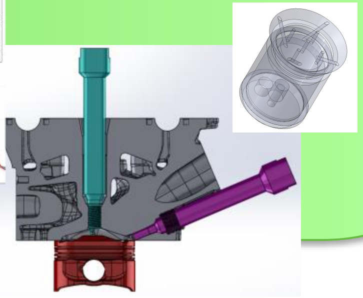


Model Integration and Validation

Improved predictive simulation of cold-start in LD GDI engines
B.02.01 (PI: Edwards, ORNL)







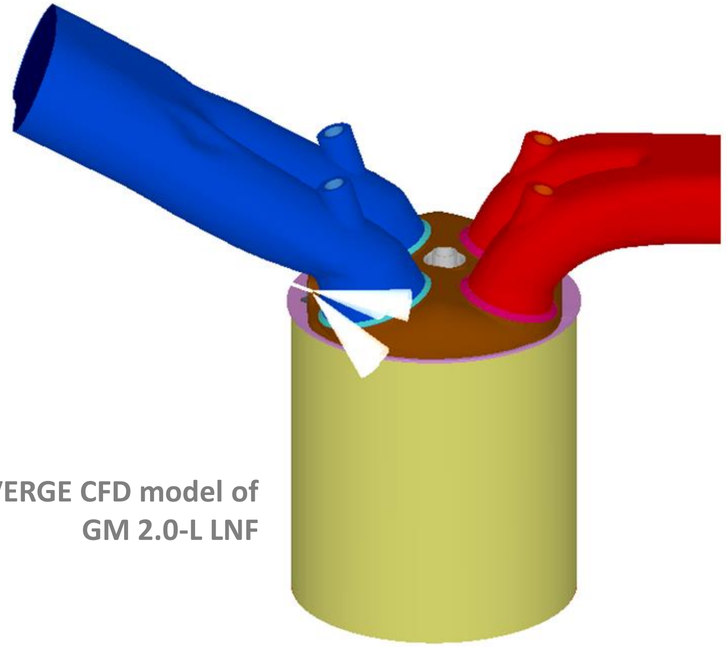
Technical Accomplishments: Baseline model development

PI: Edwards, ORNL

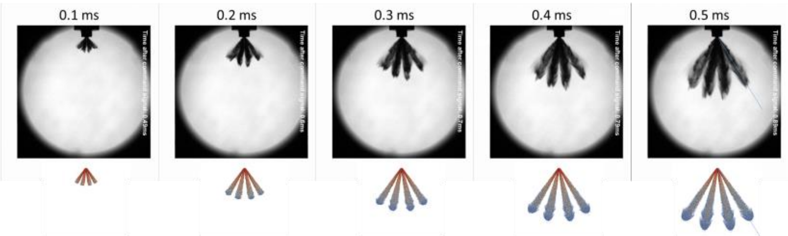
Developed CFD model to provide baseline for conventional modeling approaches

- **Moderately refined grid**
  - 2-mm base grid with refinements (to 0.25 mm) along cylinder walls, spray, and spark
  - Adaptive mesh refinement (to 0.25 mm) for velocity, temperature, and species (OH)
  - ~2.5M max cell count
- **Combustion**
  - SAGE kinetics with multi-zone chemistry (no reliance on flame-speed tables)
  - Skeletal iso-octane mechanism (38 species, 59 reactions)
  - Chemistry calculations continue past EVO and into exhaust manifold
  - Hiroyasu soot model, NOx (GRI 3.0) included in mechanism
- **RANS RNG k-ε turbulence model**
- **Constant, uniform wall temperatures**
- **Injector and spray**
  - Geometry settings and validation performed by ANL based on measurements with stock injector by SNL at ambient conditions
  - Trapezoidal injection profile with duration calculated to provide desired injection pressure
  - Conventional submodels: ***Frossling evaporation, blob distribution, KH-RT breakup, NTC collisions, dynamic drop drag, O'Rourke film/splash***

Walltime per cycle: ~36 hrs on 72 CPU cores



CONVERGE CFD model of GM 2.0-L LNF



Comparison of predicted spray shape and penetration with SNL imaging

Courtesy: ANL

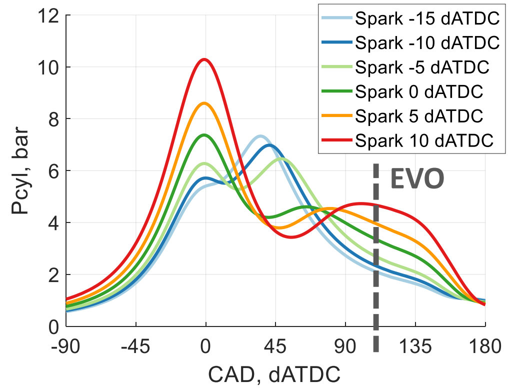
Technical Accomplishments: Comparison to experiments

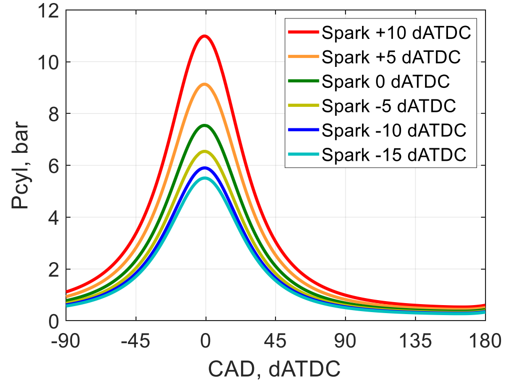
- **Baseline model results compared to experiments under ACEC Tech Team Cold-Start Protocol** (ACE 149, Curran)
    - Single-cylinder version of GM 2.0-L LNF engine at ORNL using RD5-87 gasoline reference fuel
    - ACEC Cold-Start Protocol, catalyst heating mode:
        - Steady state at 1300 rpm, 2-bar nIMEP (controlled with fuel and throttle)
        - Stoichiometric fueling (exhaust measurement) with ***spark timing swept to vary exhaust enthalpy***
        - ***20°C intake air, engine-out coolant, and engine-out oil temperatures***
    - Combustion occurs late in cycle and continues past EVO (and likely into exhaust manifold)
    - High cyclic variability, especially for earliest spark timings

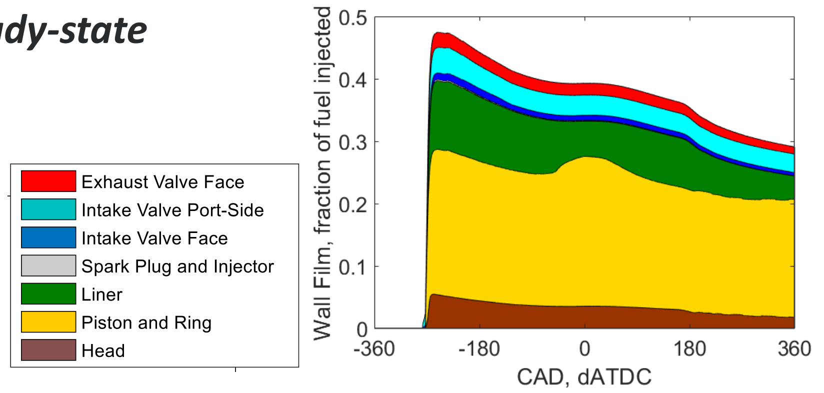
As expected, baseline model fails to fully capture observed combustion performance

- **For 20°C cold-soak conditions, the model predicts no combustion**
    - *Fuel fails to evaporate with almost 50% of injected fuel forming wall film*
    - ***However, these conditions are more representative of first-crank than the steady-state conditions of the experiments***

Need improved understanding of actual thermal conditions in engine





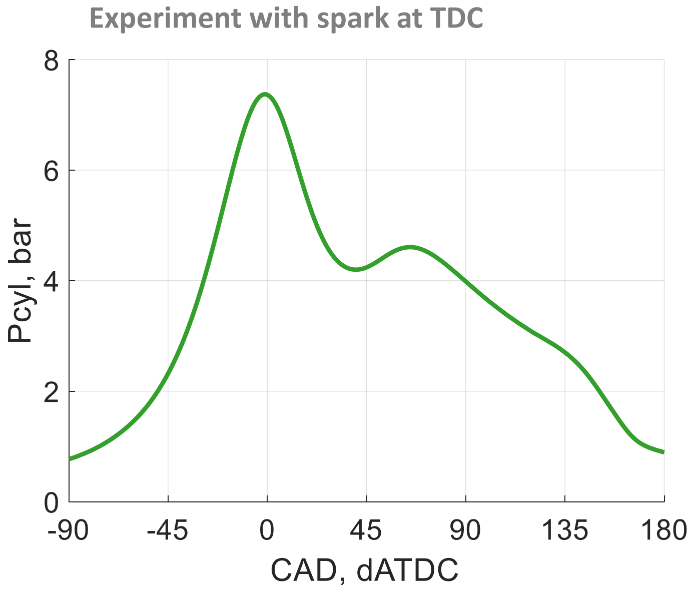


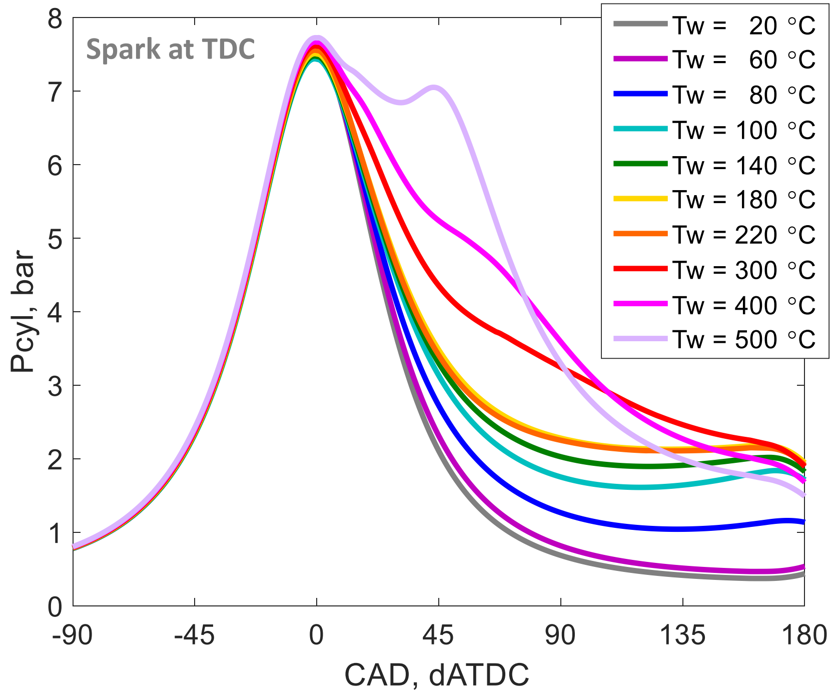
Technical Accomplishments: Sensitivity to thermal BCs

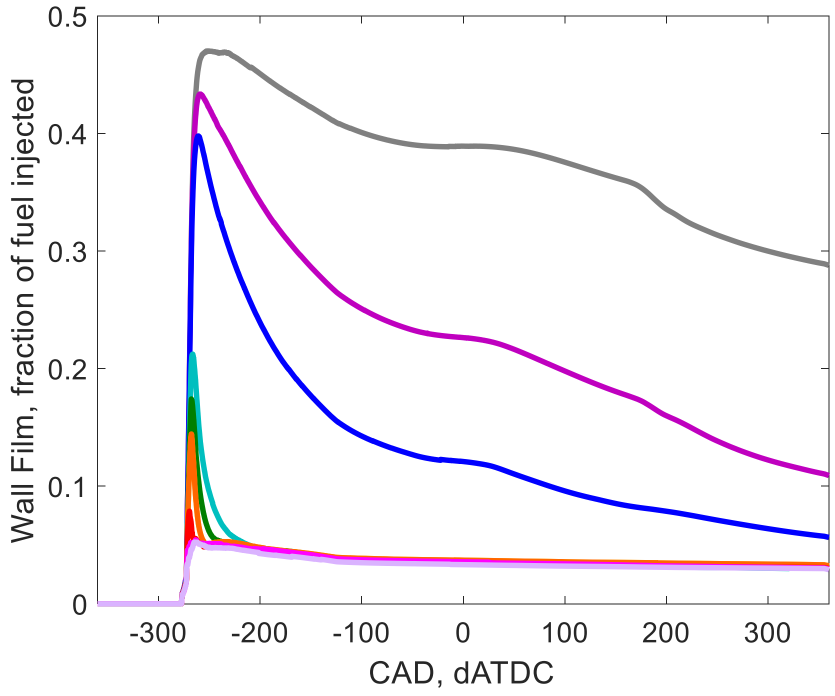
PI: Edwards, ORNL

- **Cylinder wall temperature sweep performed to evaluate sensitivity to thermal BCs**
  - No combustion noted for wall temperatures below ~60°C
  - Highly sensitive up to ~180°C as wall-film evaporation increases
  - Low sensitivity above ~180°C, remaining wall film forms within intake port (20°C)
  - High wall temperatures promote more complete burn

Additional factors also likely impacting the model accuracy.







Technical Accomplishments: Sensitivity to evaporation

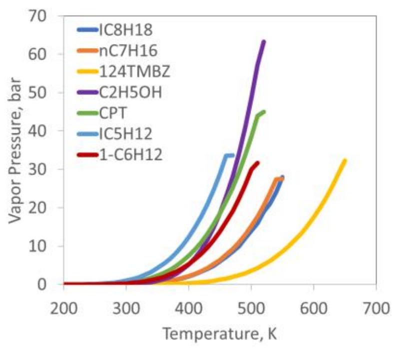
PI: Edwards, ORNL

- **Simulations with PACE RD5-87 surrogate show strong preferential evaporation**
  - Multicomponent fuel
  - Frossling evaporation with boiling
  - Pre-combustion, spark at TDC
- ***<u>Predicted composition of fuel vapor and remaining liquid in parcels and film vary considerably from surrogate formulation</u>***
  - Very sensitive to thermal conditions

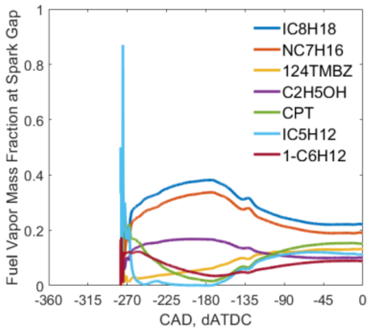
Need to validate and/or improve model predictions for evaporation

Surrogate Component	Mass %
1,2,4-trimethylbenzene	30.11
iso-octane	19.89
n-heptane	17.13
cyclopentane	10.6
ethanol	9.95
iso-pentane	6.35
1-hexene	5.97

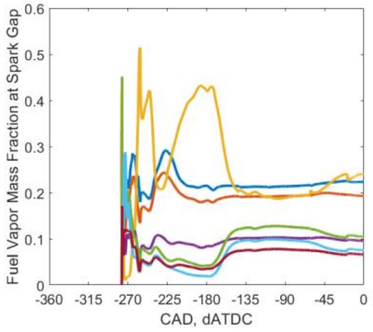
ACE 139, Wagnon



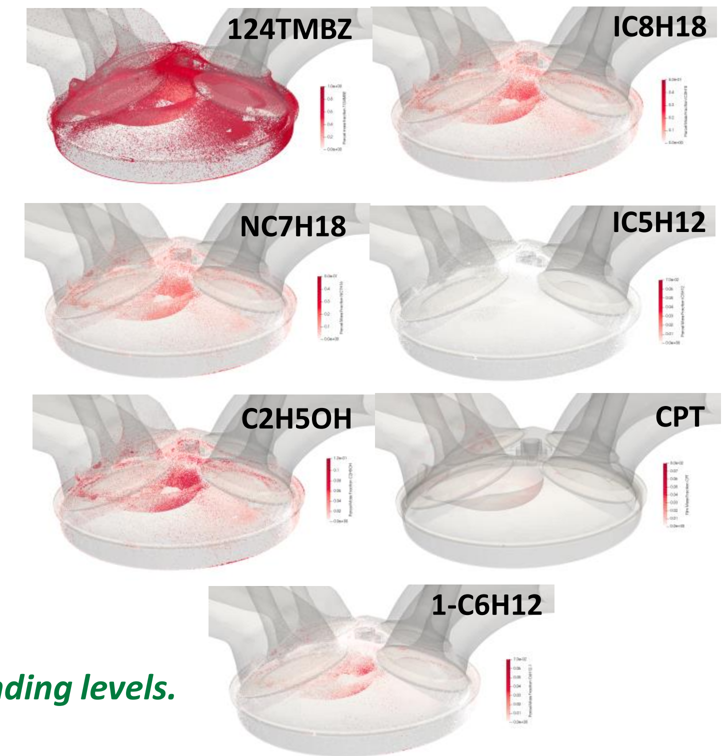
Tw = 20°C



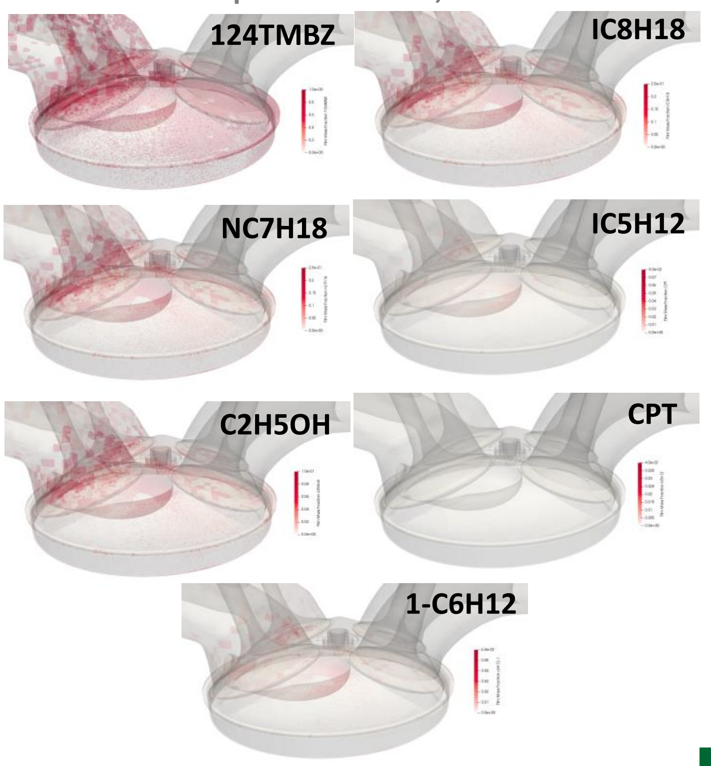
Tw = 100+ °C



Parcel composition at TDC, Tw = 20°C



Film composition at TDC, Tw = 20°C



<u>Remaining and Future Work</u>

- **Compare with free-spray and film experiments at cold-start conditions**
- **Implement Corrected Distortion spray model with flash boiling model**
  - PI: Nguyen, SNL (ACE 144, Pickett)

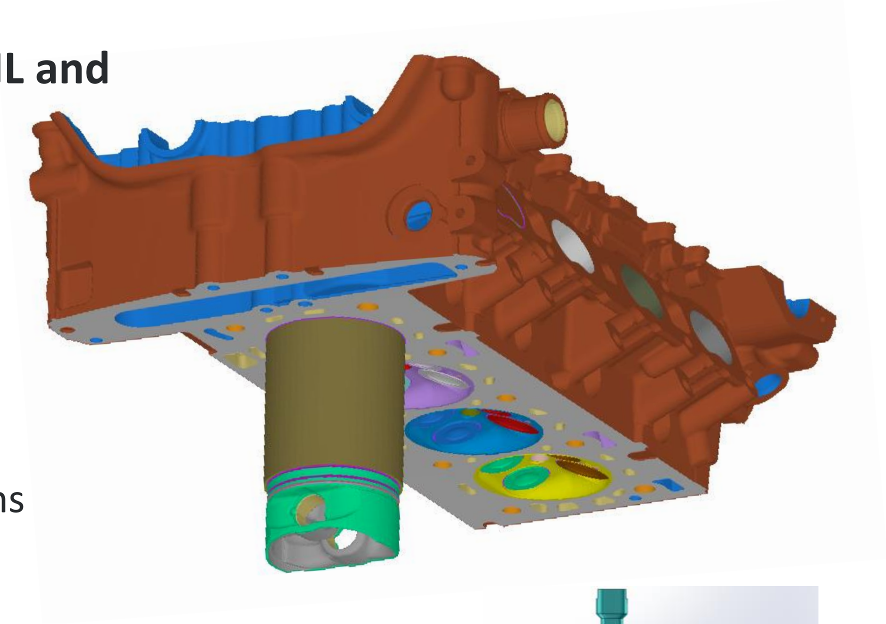
Any proposed future work is subject to change based on funding levels.

Technical Accomplishments: CHT modeling

PI: Edwards, ORNL

Coupled conjugate heat transfer (CHT) model to determine thermal BCs

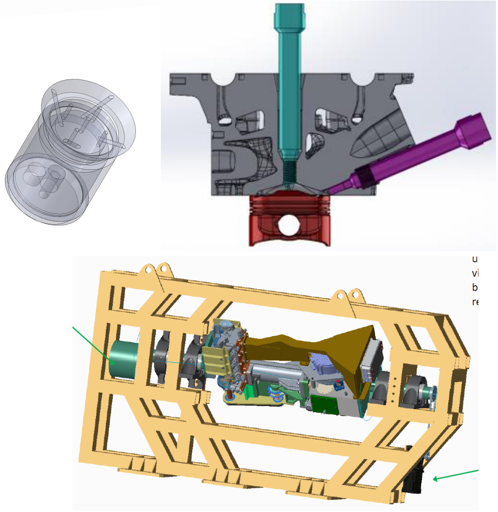
- **3-D CHT model of the full multi-cylinder engine has been developed by ORNL and Convergent Science**
  - Based on CT scans of engine (head, piston, liner)
  - Exhaust manifold will also be added
  - Completes FY20 Q1 milestone
- **Model will provide spatially and temporally varying BCs**
  - ***Need improved measurement of thermal BCs in engines for validation***
  - Multiple approaches under development within PACE and other DOE-VTO programs



Remaining and Future Work

- **Simulations with coupled CHT planned to begin in Spring 2020**
  - Initial conditions from wall temperature sweep case that burns
  - Optimum spray submodel settings
  - Submitted 2020 ALCC proposal for Summit to help support this effort
- **Simulation of reference case to compare CONVERGE and FEARCE CHT approaches**
  - Non-reacting flow over plate
  - Coordinating with LANL

Multiple approaches being used at ORNL to acquire thermal BC data for validation



Any proposed future work is subject to change based on funding levels.

Approach: Improving experimental measurement of thermal BCs

Accurate measurements of thermal BCs and their impacts are needed to develop and validate heat transfer models

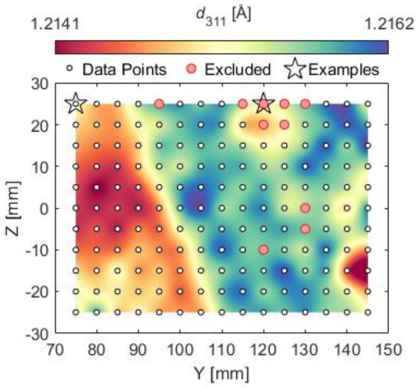
- **Multiple approaches under development within PACE and other DOE-VTO programs (e.g., HD Consortium)**

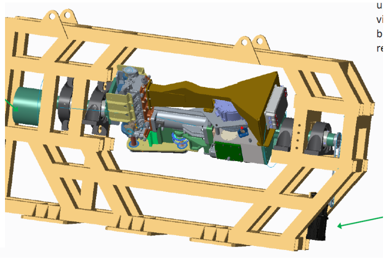
Neutron diffraction for *in situ* measurements in an operating engine
B.01.01 (PI: Wissink, ORNL)

Approach:
- Neutron diffraction to measure lattice strain in metal engine components
- Strain provides stress and temperature
- Measurements from operating engine with VULCAN diffractometer at ORNL's Spallation Neutron Source (SNS).

Objectives:
- Temporal and spatial temperature measurements throughout metal parts of operating engine

Outcomes:
- New understanding and validation data for model development



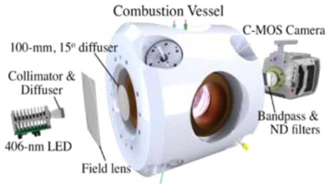


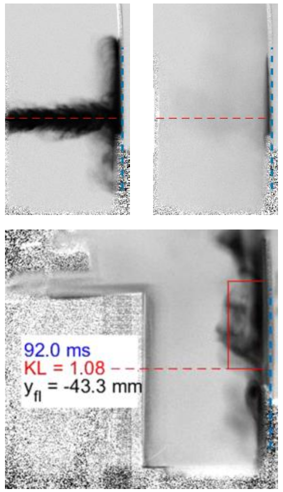
Spray-wall impingement with film formation and soot quantification
D.01.05 (PI: Pickett, SNL), D.01.04 (PI: Manin, SNL *rest of* FY20)

Approach:
- Optical spray-chamber measurements of spray-wall impingement and film formation
- Premixed reactants ignited to observe soot formation from burning film
- Adding capability to control wall temperature

Objectives:
- Optical measurements of thermal impact on film development and soot formation from burning film

Outcomes:
- New understanding and validation data for model development





This presentation focuses on cold-start applications, but successful efforts will impact all engine operation modes

Approach: Neutron diffraction for in situ measurements in an operating engine

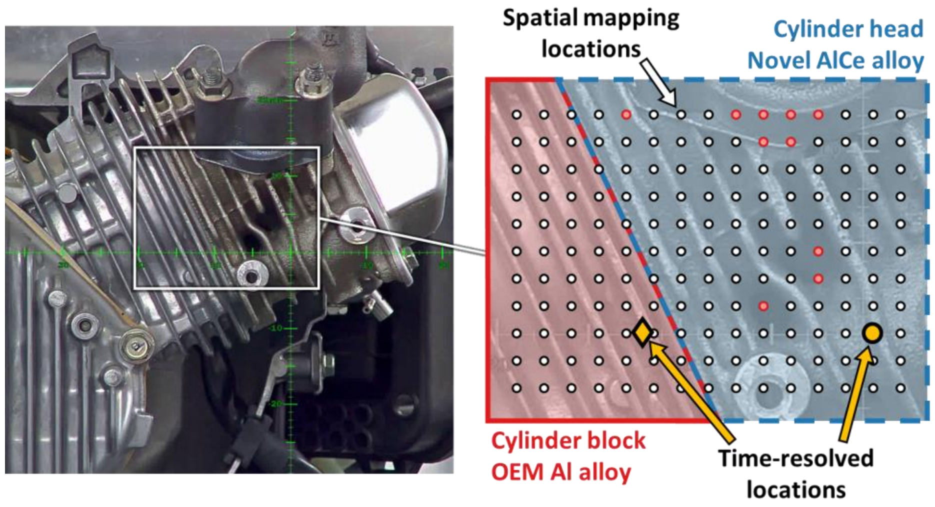
PI: Wissink, ORNL

- **Experimental thermal BC data for validation of high-fidelity engine models is sparse or non-existent**
  - Current state of the art: Fast-response thermocouples
    - Invasive, complex machining, durability concerns, point measurement, low time resolution
  - Many assumptions and tuning constants required to match measured point data
    - Only predictive in well-understood system under limited scope

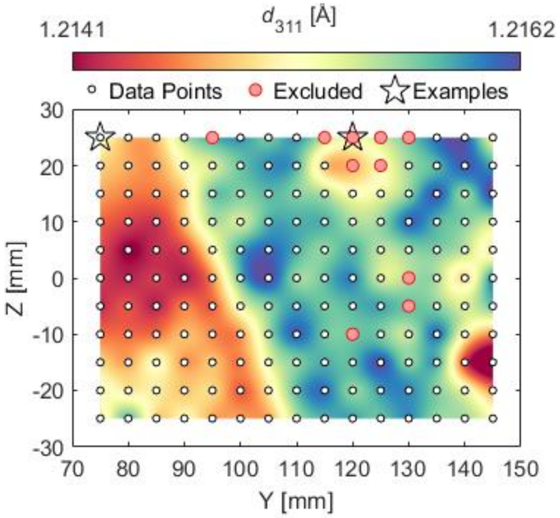
- **True volumetric measurements with neutron diffraction at the Spallation Neutron Source**
  - Neutron diffraction can directly measure **lattice strain** inside bulk materials
  - With known material properties, this can tell you both the **temperature** and **stress** throughout the entire volume of a part
  - Can be done under **dynamic conditions**, and even in **moving parts**

Prior work: Proof-of-concept measurements from cylinder head of a running small engine at SNS VULCAN

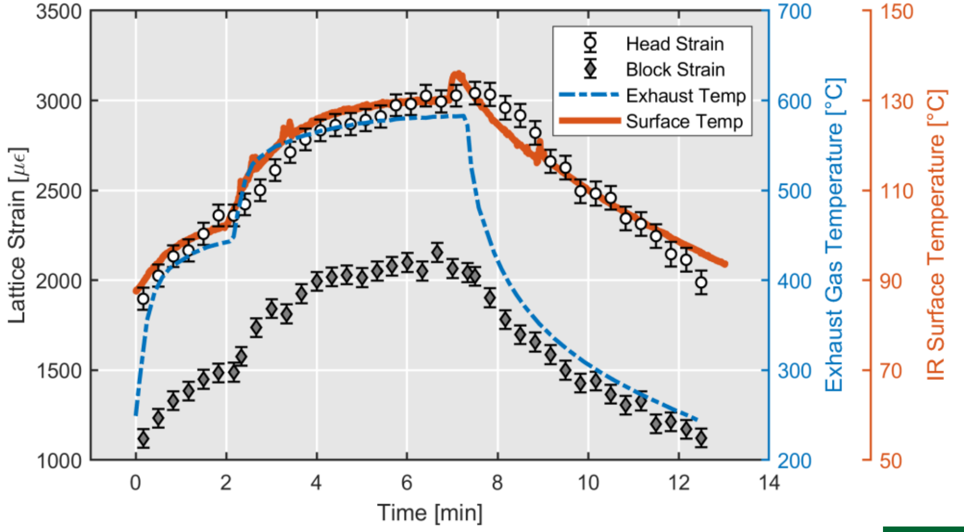
Real components



Spatial mapping



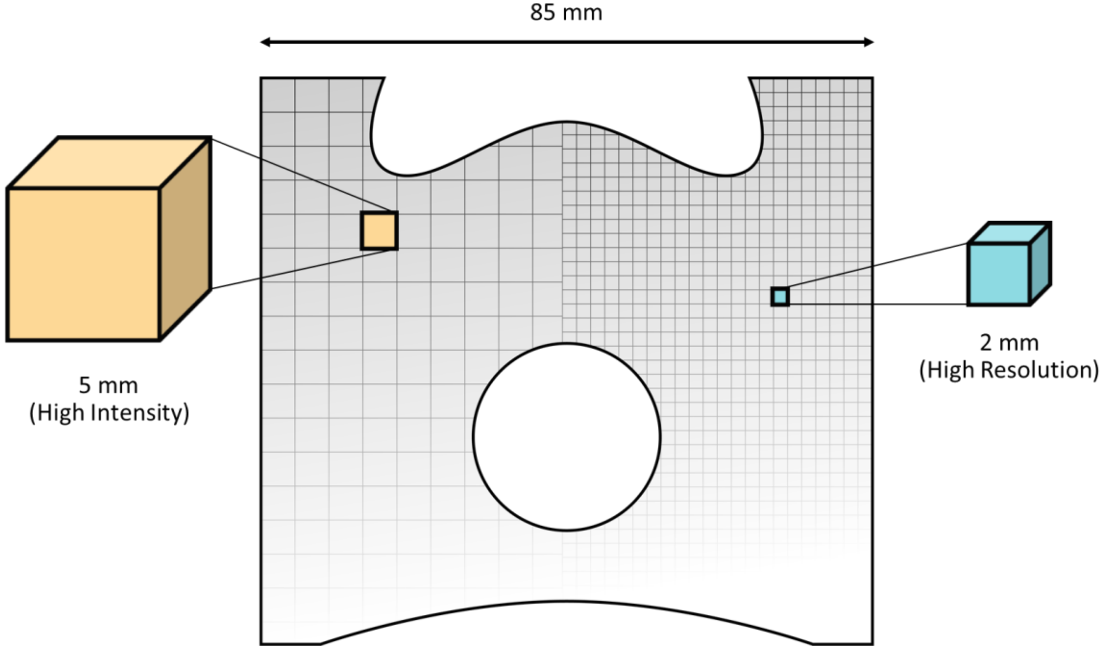
Time-resolved mapping



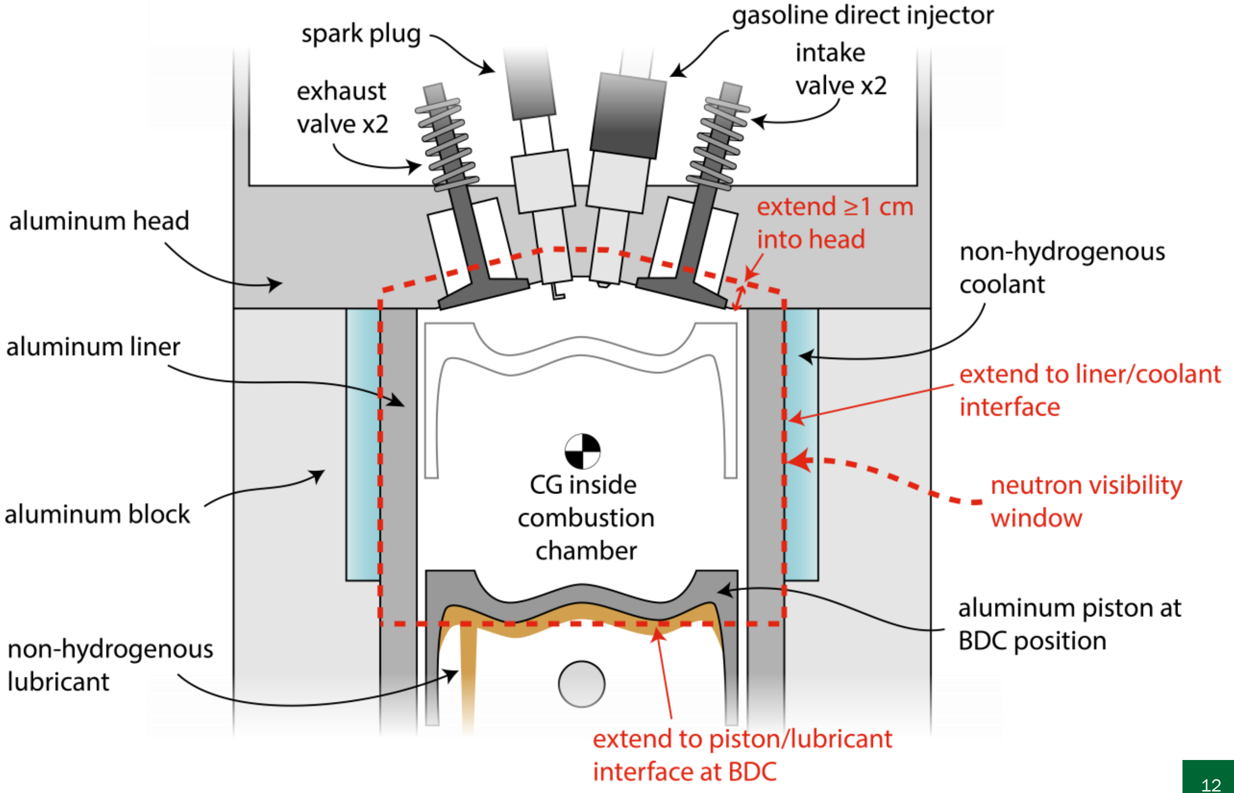
Approach: Neutron diffraction for in situ measurements in an operating engine

PI: Wissink, ORNL

- Neutron diffraction targets a "gauge volume" of predefined size inside the sample
- Entire volume of a sample can be scanned by moving it through the neutron beam
- Gauge volume sizes available at the SNS Engineering Materials Diffractometer (VULCAN) are appropriate for automotive geometry



- Developing purpose-built "neutronic engine" to enable time-resolved neutron diffraction measurements of combustion chamber thermal boundary conditions
- Goal is to create a measurement region for neutron diagnostic which encompasses all of the solid metal volumes in direct contact with combustion chamber

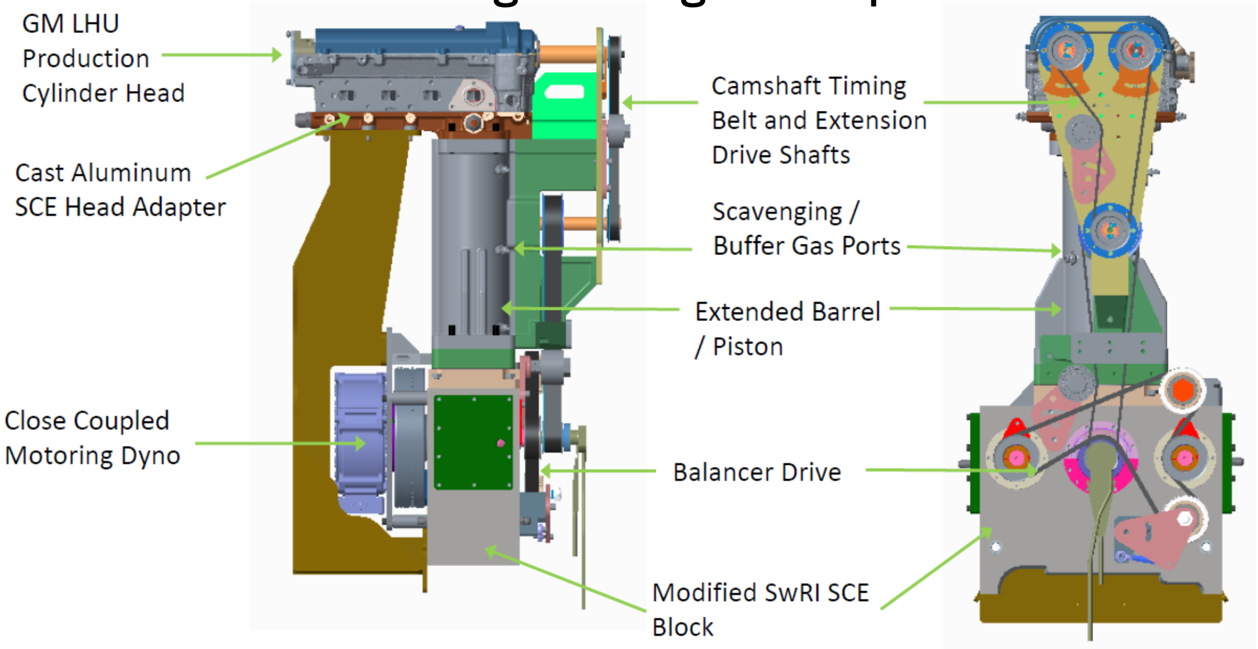


Technical Accomplishments: Neutronic Engine Design Addresses Unique Challenges

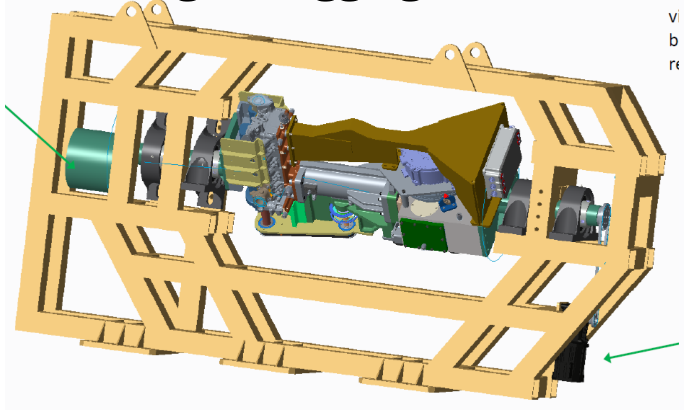
PI: Wissink, ORNL

- **Engine details:**
  - Single-cylinder based on production GM LHU cylinder head and SwRI bottom end
  - 86 mm bore x 86 mm stroke, 4 valve, side mount DI
  - Representative of modern SI engine, retains stock combustion chamber geometry, aligns well with existing engine platforms at ORNL (GM LNF)
  - Fluorocarbon-based coolant and lubricant for improved neutron visibility
- **Subcontract issued to Southwest Research Institute (SwRI) to design and build engine, meeting Sept 2019 milestone for engine requisition**
  - Midpoint Design Review completed; Phase 2 of design currently in progress
  - Delivery originally scheduled for Fall 2020, may be impacted by COVID-19
- **Assembly packaging**
  - Engine and close-coupled dyno mounted horizontally in rigging frame with rotational mounts
  - Fits within sample space at VULCAN instrument

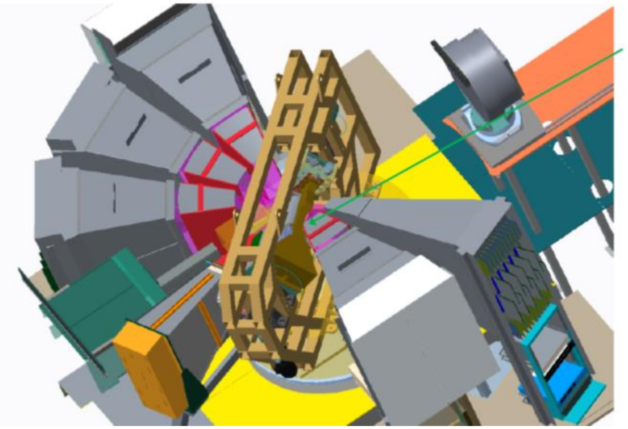
Engine Design Concept



Engine Rigging Frame

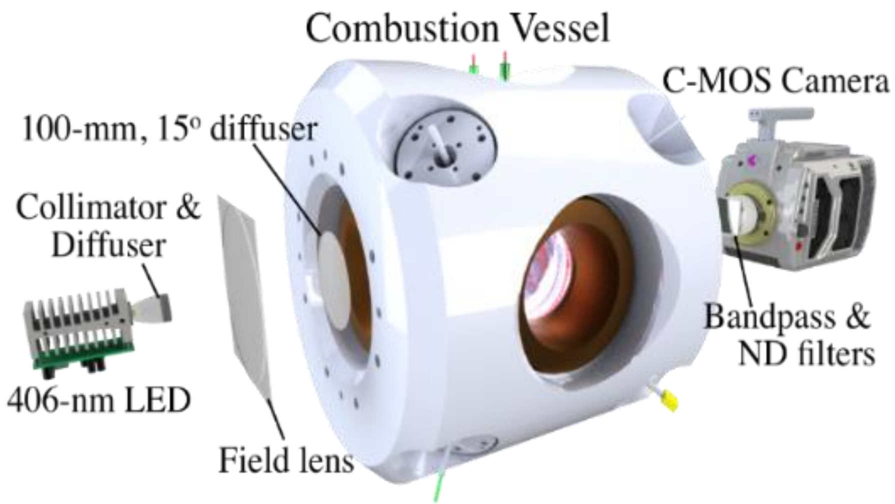


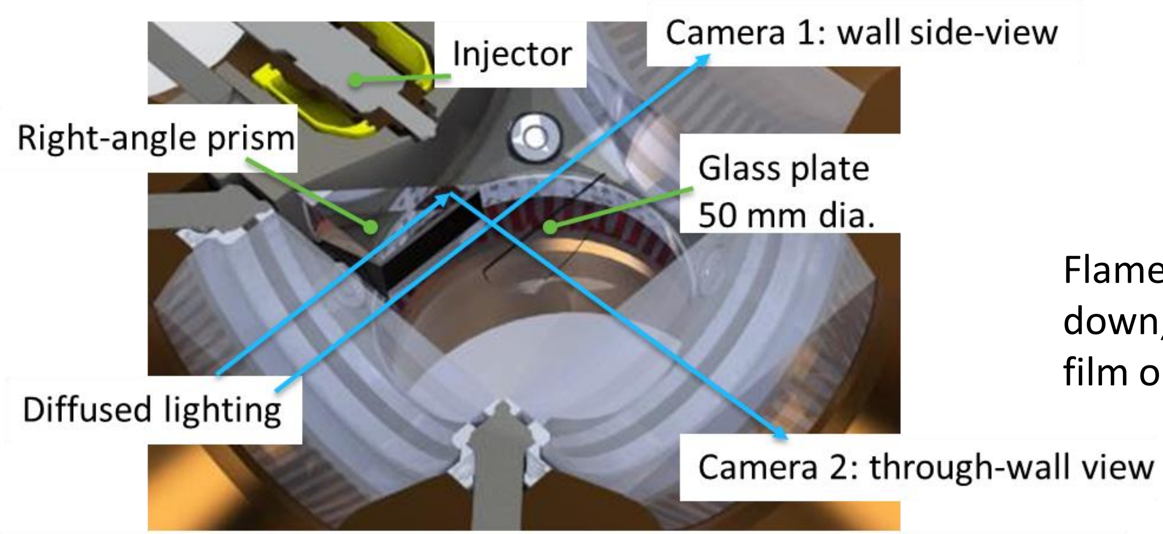
Installation at VULCAN



Approach: Spray-wall impingement, combustion, and soot quantification (from wall film)

PIs: Pickett & Manin, SNL

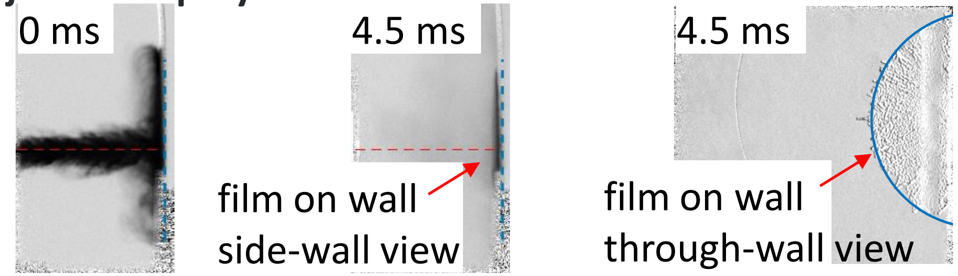




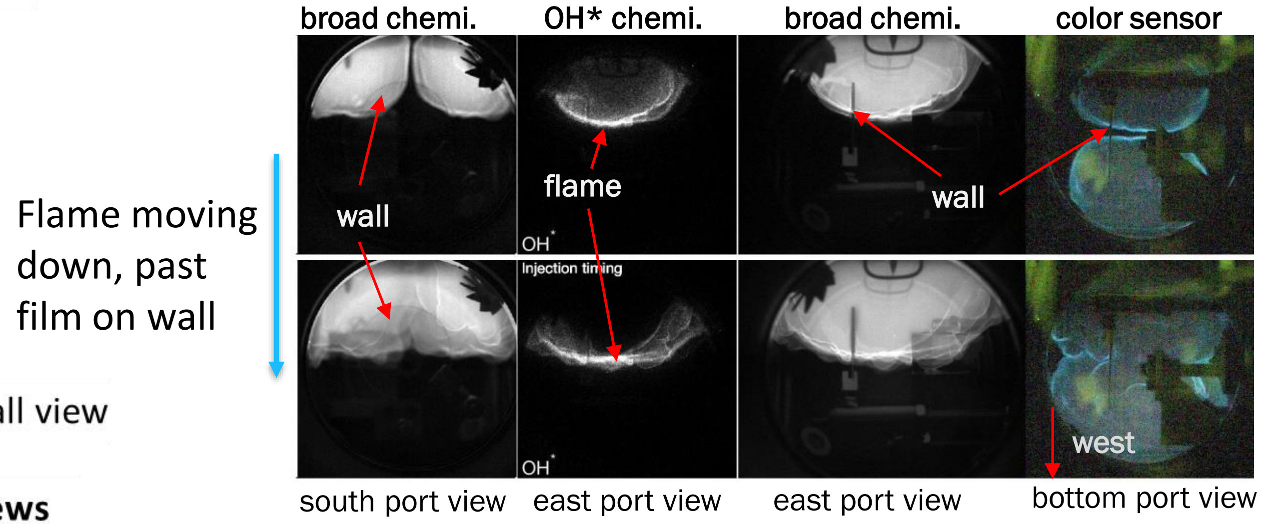
Simultaneous extinction imaging for soot (and liquid) in two views

Steps of film combustion experiment:

1. **Prepare chamber with stoichiometric reactants in chamber**
2. **Spark ignite at two locations at top of chamber**
3. **Inject fuel spray to form film on flat wall at x = 50 mm**



4. **Observe flame passing over film, in analog to engine combustion with films on surfaces**



5. **Quantify soot formation in simultaneous lines of sight "along" wall and "through" wall**

Technical Accomplishments: Wall-film soot is very sensitive to wall temperature

PIs: Pickett & Manin, SNL

- **102 °C wall T compared to 110 °C wall T optical thickness:** $\int_{-z}^{-z} f_v(z)\frac{6\pi}{\lambda}(1+\alpha_{sa})E(m)dz = KL$
  - 6.7 x 16.4 mm region for mean KL at upper portion of film
  - Time relative to flame passing CENTER of film; flame position (from OH* and measured P)
  - Smaller liquid film prior to the flame with only 8 °C higher wall temperature
  - No measurable soot until AFTER flame passes
  - Soot forms AWAY from wall (in high T gases) and grows as T & P increase
- **Much higher mean optical thickness with slightly lower wall temperature**

Wall temperature and gas temperature in boundary layer are critical!

Injector conditions

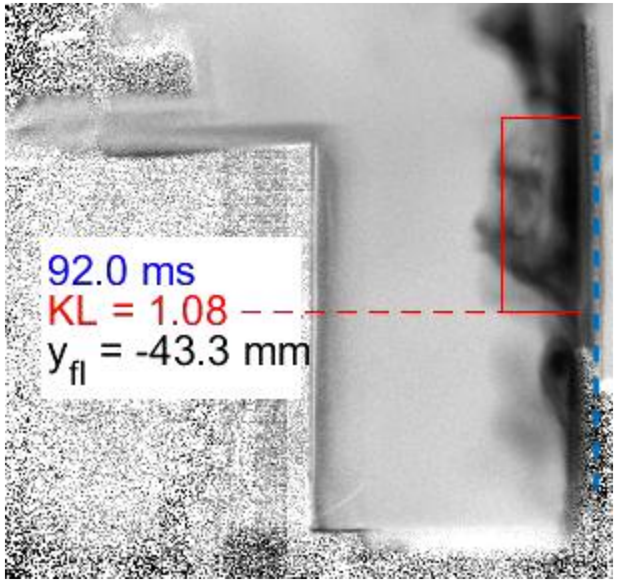
Fuel	**RD-587**
10% ethanol PACE gasoline	
Inj Pressure	350 bar
Inj Duration	2.4 ms
Inj Mass	13 mg
Injector nozzle	single-axial
Nozzle diam.	0.189 mm

Ambient conditions

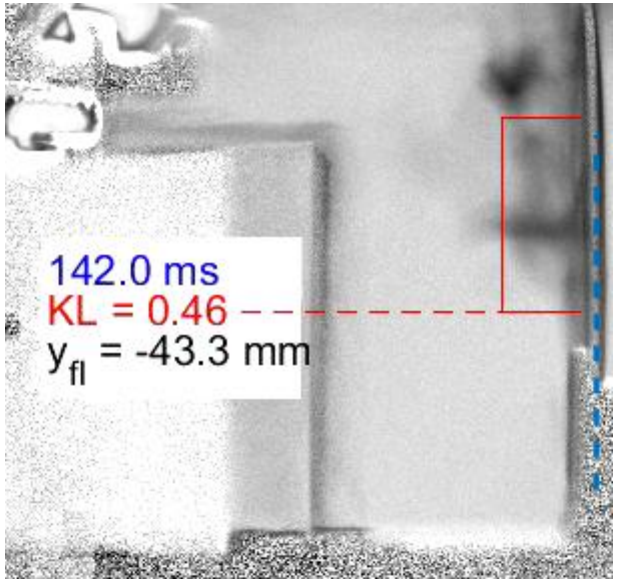
C2H2	3.2 v%
H2	0.5 v%
O2	8.2 v%
N2	13 v%
equiv. ratio	**stoich. dilute**
Initial P	7.0 bar

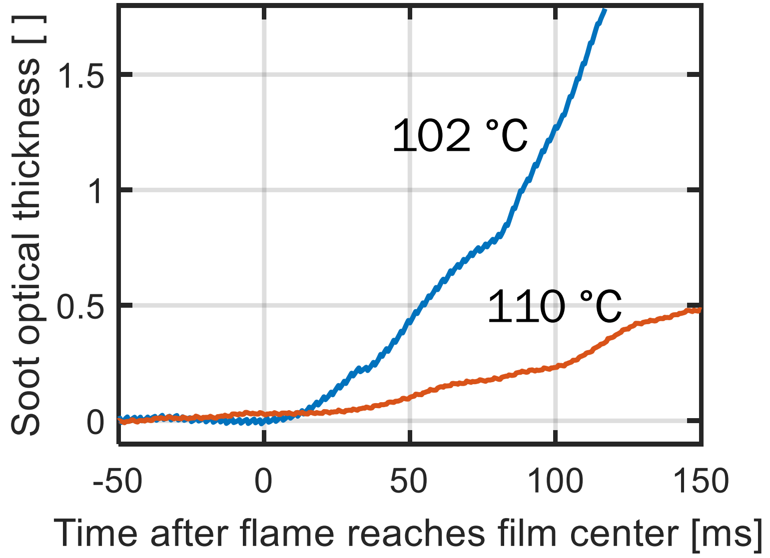
- Wall temperature must be controlled in any impingement experiment!
- Modeled wall temperature should be considered with great concern!

102 °C wall T



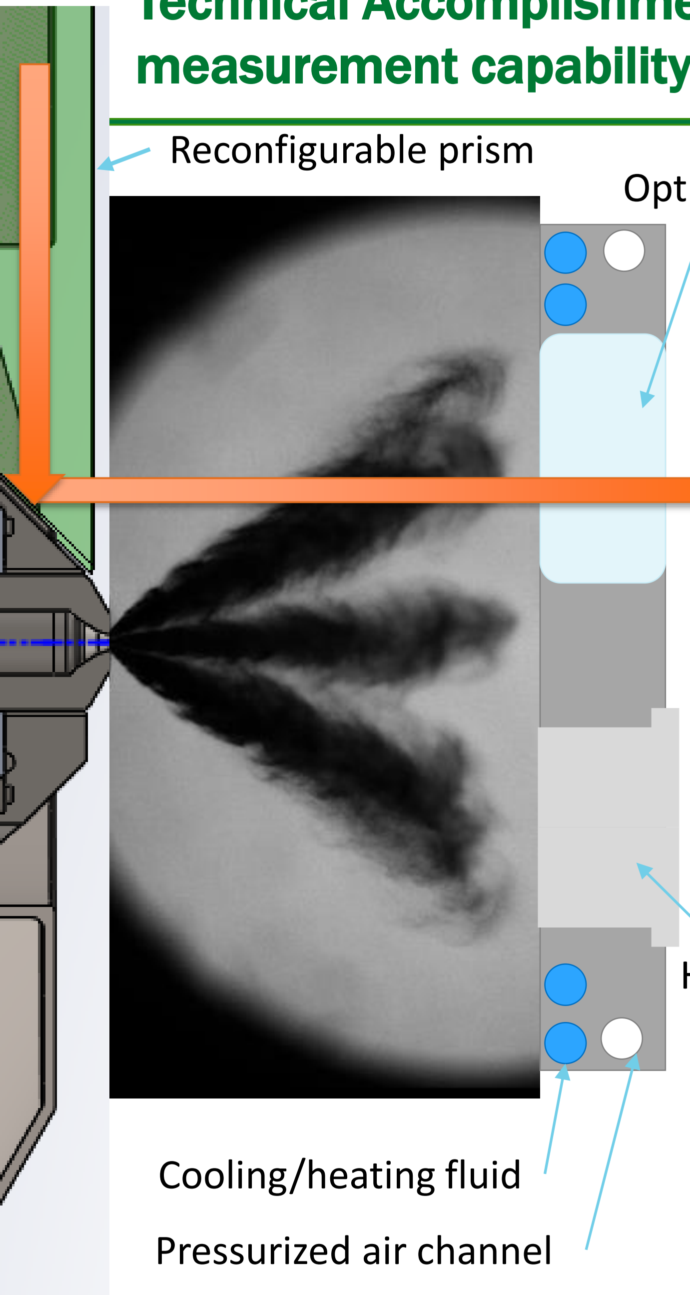
110 °C wall T





Technical Accomplishments: Designed wall apparatus with precise temperature control and heat-flux measurement capability

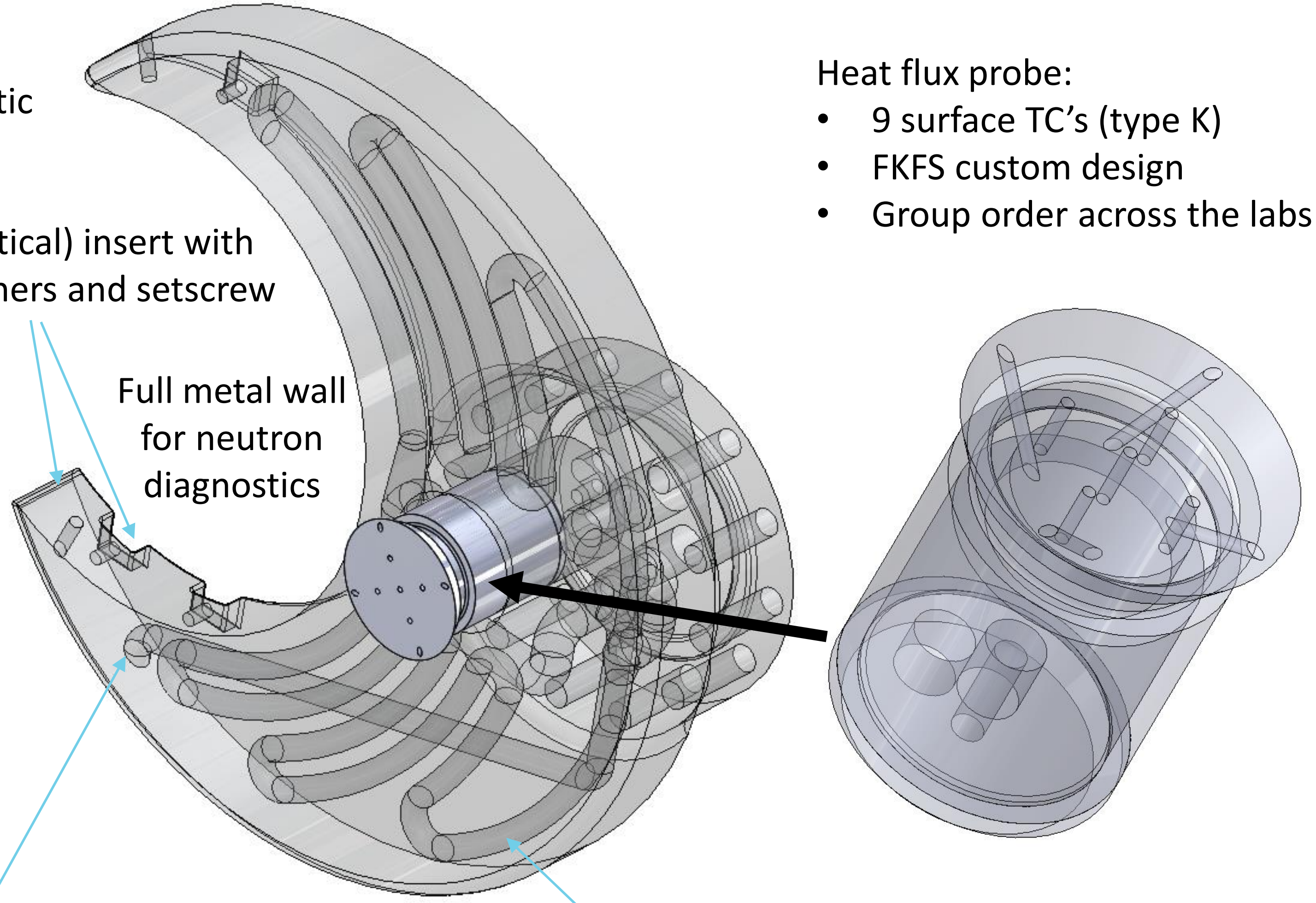
PIs: Pickett & Manin, SNL



D.01.05
Pickett, SNL

D.01.02
Wissink, ORNL

3D printed wall allows for inner geometry



Heat flux probe:
- 9 surface TC's (type K)
- FKFS custom design
- Group order across the labs

Milestones

Date	PI	Milestone	Status
FY2019 Q4	Wissink, ORNL	Submit requisition for engine design and fabrication.	**MET**
FY2019 Q4	Pickett, SNL	Quantify soot formation from burning fuel films under stoichiometric operation.	**MET**
FY2020 Q1	Edwards, ORNL	Develop new full-engine CFD model with CHT for cold-start efforts.	**MET**
FY2020 Q3	Wissink, ORNL	Finalize design elements for engine and support systems.	On Track
FY2020 Q4	Pickett, SNL	Commission temperature-controlled wall for film and combustion experiments in spray chamber	On Track
FY2020 Q4	Edwards, ORNL	Perform assessment of state-of-the-art cold-start modeling approaches to identify key gaps and needs.	On Track

Remaining FY20 and Proposed Future Work

- **Edwards: Improved predictive simulation of cold-start in LD GDI engines**
  - Complete baseline model development and remaining sensitivity studies
  - Comparison of CHT approaches for CONVERGE and FEARCE for non-reacting reference case
  - CHT full-engine simulations at cold-start conditions
  - Implement SNL Corrected Distortion spray submodel with boiling
  - Implement additional submodels as they become available
  - Implement modeling for additional engines and test facilities including future PACE common engine platform for validation
- **Wissink: Neutron diffraction for in situ measurements in an operating engine**
  - Commission engine and perform first diffraction measurements
  - Align target operating conditions for volumetrically-resolved thermal boundary condition measurements with modeling tasks
- **Pickett & Manin: Spray-wall impingement with film formation and soot quantification**
  - Install temperature-controlled wall and heat flux probe in combustion vessel and flow spray chamber
  - Soot film experiments and pyrolysis with variation in ambient oxygen concentration (0 – 3%)
  - Soot measurements from non-wall sources, such as dribble at the end of injection
  - Provide quantitative pyrolysis and soot film data to PACE modeling partners

Any proposed future work is subject to change based on funding levels.

Remaining challenges and barriers

Overall challenges and barriers for PACE program are covered in ACE 138

- **Edwards: Improved predictive simulation of cold-start in LD GDI engines**
  - Integration of various submodels into CONVERGE and evaluating any potential unintended interactions
  - Accurate prediction of emissions is challenging even under normal operation
- **Wissink: Neutron diffraction for *in situ* measurements in an operating engine**
  - Management of neutronic engine design, build, and commissioning
  - Integration of neutronic engine and specialized support systems into the VULCAN beamline
  - Development of techniques for spatiotemporal alignment and binning of engine and diffractometer data to enable time-resolved measurements in moving parts
- **Pickett & Manin: Spray-wall impingement with film formation and soot quantification**
  - Quantification of film thickness at stages of injection and during combustion
  - Speciation of film composition using multi-component fuel surrogate
  - Quantification of gas temperature and mixture concentration in proximity to wall and film

Responses to previous reviewer comments

Specific tasks in this presentation are new efforts that have not been reviewed previously.

- **Past reviewer comments on similar CHT simulation efforts have expressed interest in application to cold-start and the need for improved validation of the predicted thermal BCs**
  - PACE objectives and work plan were developed with these considerations in mind
    - Several tasks under PACE (and elsewhere in DOE-VTO) are developing and/or applying approaches for improved experimental measurement of thermal BCs and understanding of their impact on physics
    - PACE Major Outcome 8 specifically targets improved understanding and predictive simulation of cold start

Collaborations and Acknowledgements

PACE is a DOE-funded consortium of 6 National Labs collaboratively working toward common objectives

Overall PACE objectives and work plan were developed with input from key stakeholders including DOE, U.S. DRIVE ACEC Tech Team, and Advanced Engine Combustion (AEC) MOU members including CFD software vendors.

- **Edwards: Improved predictive simulation of cold-start in LD GDI engines**
  - Convergent Science: Support and assistance with CHT model development
  - ORNL: Experimental validation data from LNF engine
  - LLNL: Development of PACE RD5-87 surrogate and kinetic mechanism
  - SNL and ANL: Development of injector geometry and model settings from spray imaging
  - LANL: CHT comparisons for non-reacting reference case
  - GM, Convergent Science, LLNL: 2020 ALCC Cold-start proposal
  - Portions of this research used resources of the Compute and Data Environment for Science (CADES) at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.
- **Wissink: Neutron diffraction for in situ measurements in an operating engine**
  - Subcontract with SwRI to design and build neutronic engine
  - Internal collaboration with ORNL Neutron Sciences Directorate to develop facilities, sample environment, and data reduction approaches
- **Pickett: Spray-wall impingement with film formation and soot quantification**
  - Engine Combustion Network lead; ECN has chosen wall and film combustion as a topic with 20+ volunteer researchers
  - International Energy Agency soot team; Working with 6+ active institutions on problems related to soot formation in gasoline and diesel

Summary

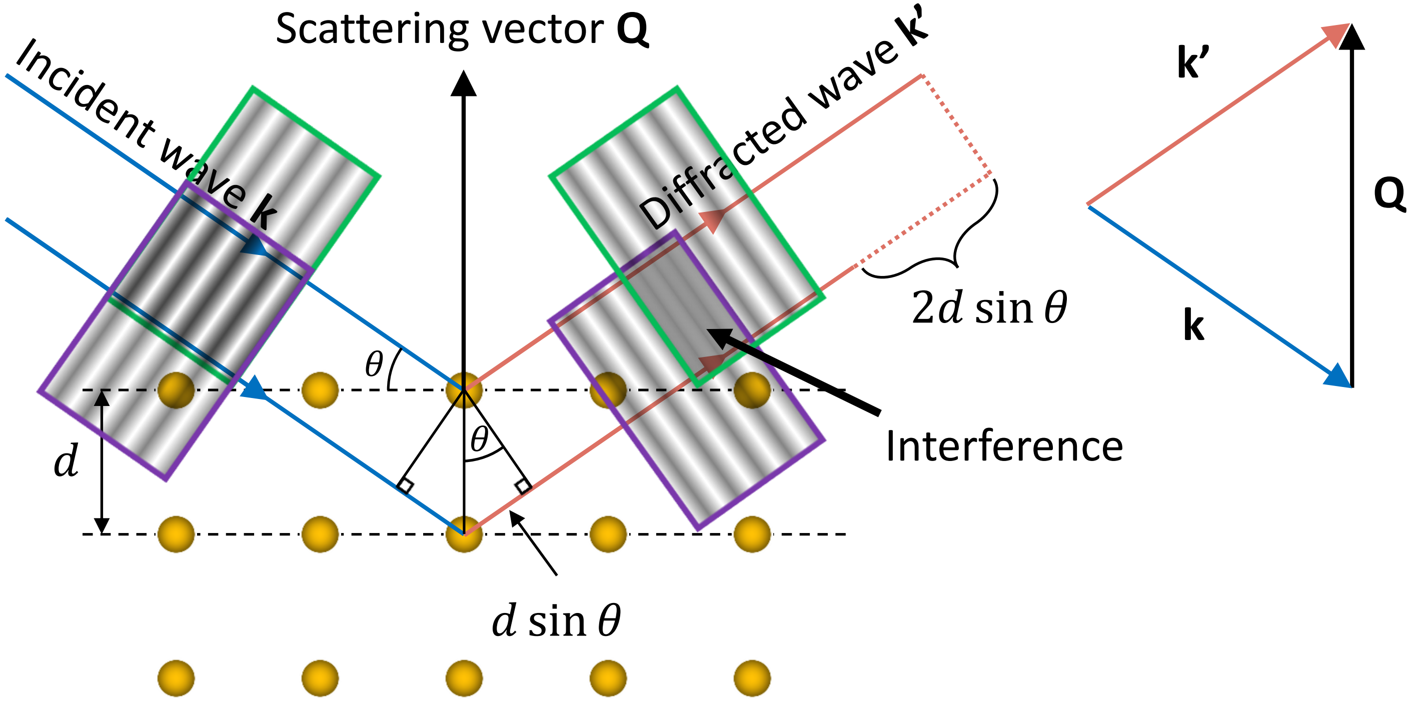
Overall summary of PACE consortium objectives and work plan provided in ACE 138

- **Relevance**
  - Addresses need for improved simulation of cold-start operation identified in U.S. DRIVE Roadmap and PACE objectives
- **Approach**
  - Experiments to provide understanding and validation data that feeds development of improved submodels and full-engine CFD
- **Technical Accomplishments**
  - Developed baseline CFD model to evaluate deficiencies and sensitivities to boundary conditions and submodel accuracies
    - Initial results show accuracy of ***thermal BCs***, ***spray models***, and ***heat transfer to and evaporation of spray and film*** are crucial
  - Design of experimental system to measure temperature throughout metal in operating LD GDI engine using neutron diffraction
    - Proof of concept previously demonstrated in working small engine
  - Design of experimental system with refined wall-temperature control to evaluate impact on spray impingement, film development, and soot formation
    - Initial results with limited thermal control show strong influence of wall temperature
- **Collaborations**
  - Strong collaboration between multiple NLs with guidance and support from industry
- **Future Work (Any proposed future work is subject to change based on funding levels)**
  - Coupled CHT simulations to refine thermal boundary conditions with comparison to experimental validation data
  - Integration of improved submodels for spray, evaporation, wall impingement, ignition, etc.
  - Commission neutronic engine and perform initial experiments
  - Install temperature-controlled wall in spray chamber and perform impingement experiments

Technical Backup Slides

Technical Backup Slides: Measuring strain with neutron diffraction

- Bragg's Law defines the condition for constructive interference when a wave is diffracted by a repeating crystal lattice
- The angle θ at which we measure the intensity of the diffracted neutrons is defined by the geometry and orientation of the detectors and collimators
- The wavelength λ of the diffracted neutrons is calculated by measuring the time of flight of the pulsed neutrons
- With the θ and λ we can correlate intensity peaks in the diffraction signal to interplanar spacing ***d***
- Spatial or temporal variations in d-spacing provide a direct measure of lattice strain within a given gauge volume at resolution <100 microstrain



Bragg's Law: $$2d \sin\theta = n\lambda$$

Lattice strain: $$\varepsilon = \frac{d - d_0}{d_0}$$

PACE PARTNERSHIP TO ADVANCE COMBUSTION ENGINES